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AN EFFICIENT METHOD FOR SOLVING STIFF TRANSIENT FIELD PROBLEMS --ETC(U)

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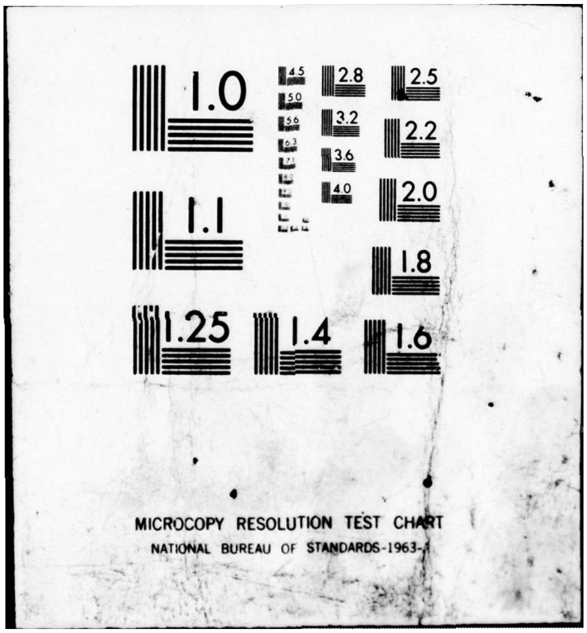

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AN EFFICIENT METHOD FOR SOLVING STIFF TRANSIENT FIELD PROBLEMS ARISING FROM FEM FORMULATIONS

Richard Franke
David Salinas

Technical Report for Period January - March 1979

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NAVAL POSTGRADUATE SCHOOL
Monterey, California

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We consider the nonlinear differential equation $\frac{\partial u}{\partial t} = L(u) + f(t)$. Use of Galerkin FEM with $u(\underset{\sim}{x}, t) \approx v(\underset{\sim}{x}, t) = \sum_{j=1}^{n} \gamma_j(t) N_j(\underset{\sim}{x})$, where the $N_j(\underset{\sim}{x})$ are specified basis functions, results in the implicit system of ordinary differential equations, (*) $\sum_{j=1}^{n} A_{ij}\dot{\gamma}_j - B_i(\gamma_1,\ldots,\gamma_n,f) = 0$, $i = 1,\ldots,n$,

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where $A_{ij} = \langle N_i, N_j \rangle$, $B_i = \langle N_i, L(v) + f \rangle$.

The method chosen for solution of stiff systems (*) is a version of Gear's method which solves the system in its implicit form. This leads to the necessity of being able to solve (repeatedly) linear algebraic equations whose coefficient matrix has the same sparse and banded nature as (A_{ij}).

Storage requirements for various orders of polynomial triangular elements under compact storage mode, profile storage mode, and banded symmetric storage mode are given and compared. For large systems (*), compact storage mode leads to significantly reduced requirements. Consideration of the linear algebraic systems which arise in Gear's method reveals that iteration should be computationally efficient. A comparison between various solution methods is given for a nonlinear reactor dynamics problem. Associated with each solution method is a different storage mode.

AN EFFICIENT METHOD FOR SOLVING STIFF TRANSIENT FIELD PROBLEMS ARISING FROM FEM FORMULATIONS*

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ABSTRACT

We consider the nonlinear differential equation $\frac{\partial u}{\partial t} = L(u) + f(t)$. Use of Galerkin FEM with $u(\underset{\sim}{x}, t) \simeq v(\underset{\sim}{x}, t) = \sum_{j=1}^{n} \gamma_j(t) N_j(\underset{\sim}{x})$, where the $N_j(\underset{\sim}{x})$ are specified basis functions, results in the implicit system of ordinary differential equations, (*) $\sum_{j=1}^{n} A_{ij}\dot{\gamma}_j - B_i(\gamma_1, \ldots, \gamma_n, f) = 0$, $i = 1, \ldots, n$, where $A_{ij} = \langle N_i, N_j \rangle$, $B_i = \langle N_i, L(v) + f \rangle$.

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Storage requirements for various orders of polynomial triangular elements under compact storage mode, profile storage mode, and banded

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symmetric storage mode are given and compared. For large systems (*), compact storage mode leads to significantly reduced requirements. Consideration of the linear algebraic systems which arise in Gear's method reveals that iteration should be computationally efficient. A comparison between various solution methods is given for a nonlinear reactor dynamics problem. Associated with each solution method is a different storage mode.

1. Discription of the Problem

We consider a nonlinear p.d.e. of the parabolic type,

$$\frac{\partial u}{\partial t} = L(u) + f \quad \underset{\sim}{x} \in D, \; t \in \tau \qquad (1)$$

with appropriate initial and boundary conditions, and L denotes spatial operators. In accordance with a weighted residual FEM formulation, an approximate solution $v(\underset{\sim}{x},t)$ in the form

$$u(\underset{\sim}{x}, t) \cong v(\underset{\sim}{x},t) = \sum_{j=1}^{n} \gamma_j(t) N_j(\underset{\sim}{x}) \qquad (2)$$

is assumed. In Eq. (2), $N_j(\underset{\sim}{x})$ are a set of specified interpolation functions with local support, and the $\gamma_j(t)$ are the solution coefficients to be determined. Setting the residual function

$$R(\underset{\sim}{x}, t) = \frac{\partial v}{\partial t} - L(v) - f \qquad (3)$$

orthogonal to each of the weighting functions $W_i(\underset{\sim}{x})$, $i = 1, \ldots, n$, i.e.

$$\langle R, W_i \rangle = 0, \; i = 1, \ldots, n \qquad (4)$$

yields the system of nonlinear o.d.e.,

$$\sum_{j=1}^{n} A_{ij}\dot{\gamma}_j - B_i(\gamma_1,\ldots\ldots,\gamma_n, f) = 0 \qquad (5)$$

with initial conditions, where

$$\left.\begin{aligned} A_{ij} &= \langle W_i, N_j\rangle \\ B_i &= \langle L(V) + f, W_i\rangle \end{aligned}\right\} \qquad (6)$$

Out objective is to select a method of solution of Eq. (5) which is efficient with respect to memory core requirement, and computational effort. With regard to core requirement, an efficient strategy should take into account the nature of the (A_{ij}) matrix. If the weighting functions have local support, A will be sparse and banded. If a Galerkin formulation is employed, $W_i = N_i$, and the (A_{ij})matrix is symmetric. In general the sparseness of (A_{ij}) increases with finer mesh discretization, as well as space dimensionality. Bandwidth and sparseness increase with higher order polynomial interpolation elements, but fewer are required to provide an accuracy achieved by lower order elements. The question of which is more efficient, higher or lower order elements, is not addressed here.

Attention is given here to a stiff system arising from a FEM formulation of a two dimensional nonlinear nuclear reactor dynamics problem [1]. Here L(u) is given by

$$L(u) = -au^2 + bu + c\Delta^2 u \qquad (7)$$

with appropriate initial and boundary conditions. In this case, Eq. (5) becomes, after an integration by parts on the Δ^2 term,

$$\Sigma A_{ij}\dot{\gamma}_j + a\Sigma\Sigma C_{ijk}\gamma_j\gamma_k - b\Sigma A_{ij}\gamma_j + c\Sigma B_{ij}\gamma_j = 0 \qquad (8)$$

where

$$\left.\begin{aligned} A_{ij} &= \langle N_i, N_j\rangle \\ C_{ijk} &= \langle N_i, N_j N_k\rangle \\ B_{ij} &= \langle \frac{\partial N_i}{\partial x}, \frac{\partial N_j}{\partial x}\rangle + \langle \frac{\partial N_i}{\partial y}, \frac{\partial N_j}{\partial y}\rangle . \end{aligned}\right\} \quad (9)$$

2. Solution Techniques for the Implicit System of O.D.E.'s

Consideration of various schemes for the solution of the implicit system of ordinary differential equations given by Eq (5) reveals that no matter what type of scheme is employed, it will involve the solution of a system of algebraic equations, possibly nonlinear if (B_i) is nonlinear. Use of even a simple scheme for explicit systems of differential equations, e.g., Euler's method, requires repeated solution of a system of linear equations with coefficient matrix (A_{ij}) for the $\dot{\gamma}_j$, given $\gamma_1, \ldots, \gamma_n$, and t. If a predictor-corrector method (or any method involving derivatives at the new time, generally called an implicit numerical method) for explicit systems of differential equations is used, a second system of algebraic equations arises for the dependent variables at the new time. Because of this second system of algebraic equations it is best to avoid having to solve (5) for derivatives by employing an ordinary diffential equation solver designed for implicit systems of equations.

Given that an implicit method will be employed to solve the system (5) there are three levels of matrix storage that are required: (1) That required by the system matrices (A_{ij}) and (B_i) (We are not being specific here about the form of (B_i); it may involve several constant matrices or may be a function of time); (2) That required by the differential equation solver; and (3) That required to represent the algebraic system of equations for $\gamma_1, \ldots, \gamma_n$ at the next time in the form required by the algebraic equation solver being used. The hierarchy of storage levels is shown schematically in Figure 1, along with possible options for differential equation solvers and algebraic equation solvers, with the preferred storage mode shown in parenthesis.

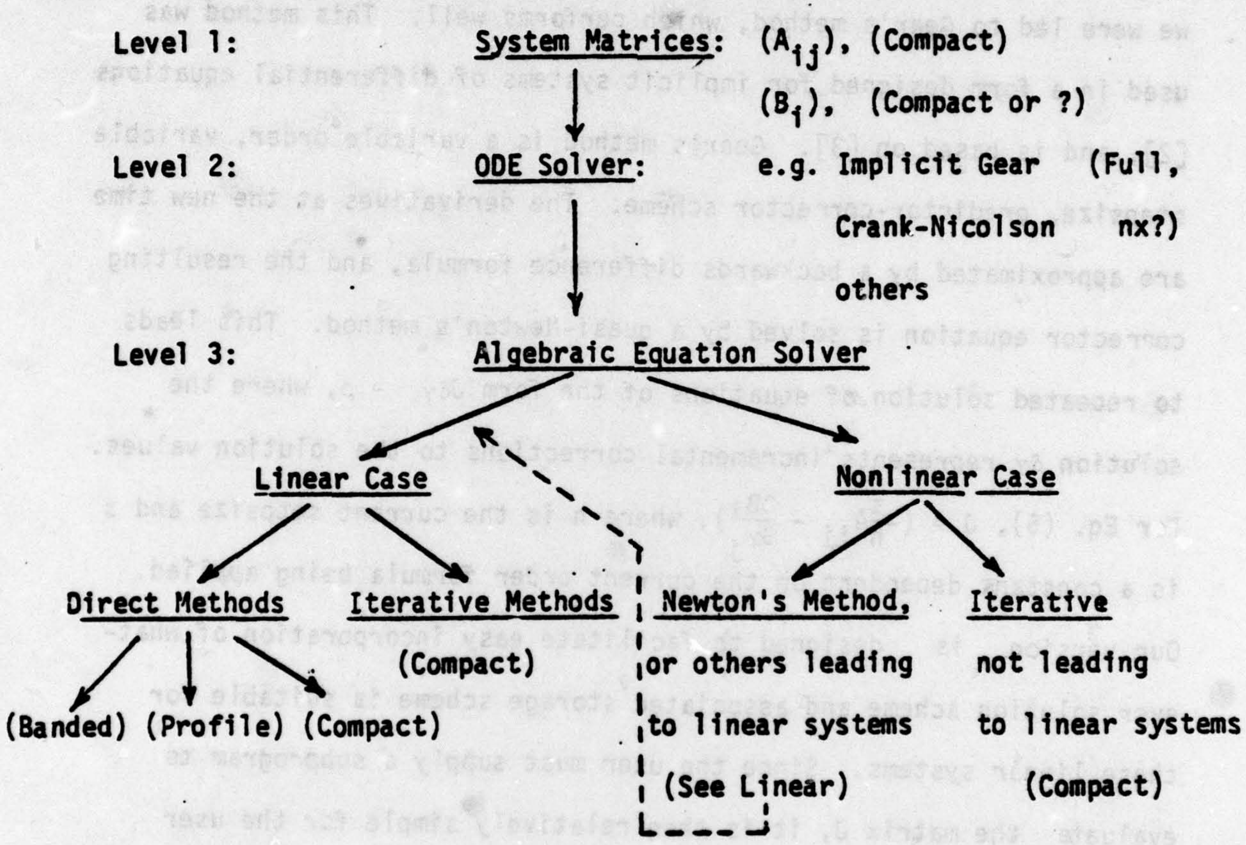


Figure 1

It is difficult to show all the possible options and Figure 1 is not meant to exclude any, but rather to emphasize several points. (1) The system matrices are used only in evaluation of the left side of (5) and can be stored in any form, some form of compact storage being efficient. (2) The differential equation solver will have its own requirements for storing the solution values, past history, and auxiliary storage.

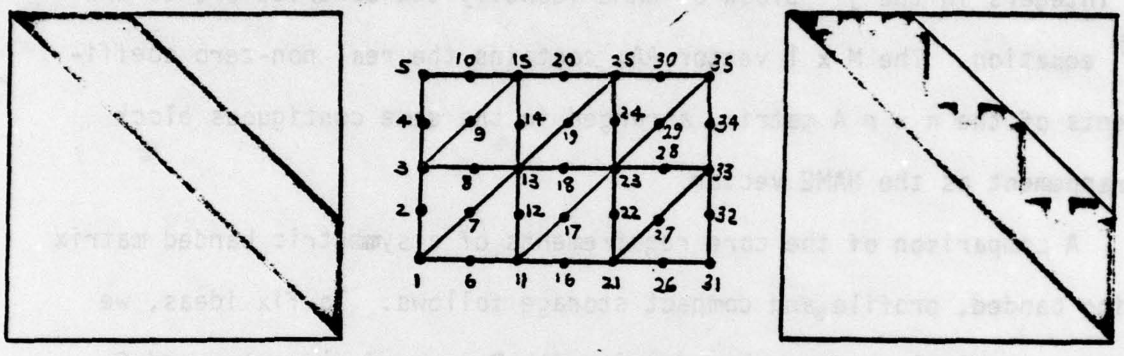
(3) The choice of solution method for the algebraic equations will determine the type of storage required at level 3. In some instances the latter choice may be determined by the differential equation solver, and could require no additional storage in some cases, but a more usual situation will be where at least one matrix must be stored.

Because the problems in which we are interested are typically stiff we were led to Gear's method, which performs well. This method was used in a form designed for implicit systems of differential equations [2], and is based on [3]. Gear's method is a variable order, variable stepsize, predictor-corrector scheme. The derivatives at the new time are approximated by a backwards difference formula, and the resulting corrector equation is solved by a quasi-Newton's method. This leads to repeated solution of equations of the form $J\delta\gamma = \rho$, where the solution $\delta\gamma$ represents incremental corrections to the solution values. For Eq. (5), $J = (-\frac{s}{h}A_{ij} - \frac{\partial B_i}{\partial \gamma_j})$, where h is the current setpsize and s is a constant dependent on the current order formula being applied. Our version is designed to facilitate easy incorporation of whatever solution scheme and associated storage scheme is suitable for these linear systems. Since the user must supply a subprogram to evaluate the matrix J, it is then relatively simple for the user to store the matrix in a form compatible with the equation solver being used.

In our scheme, the amount of storage required at level 2 is approximately 20 n words. Level 1 storage is dependent on the problem, and level 3 storage on the linear equation solver incorporated into the method. The details for a specific problem are discussed in Section 4.

3. Storage Schemes

The most common method of storing matrices in FEM, is the banded storage scheme, whereby the bandwidth (or half bandwidth in the case of symmetric matrices) terms are stored. Some reduction in storage is obtained by profile (or skyline) storage. In this scheme, some of the zero terms within the band are eliminated. Band and profile storage are schematically shown in Figure 2.



Symmetric Banded Grid (R=2, S=3, t=2) Profile

Figure 2

For large systems, the storage allocated to zero terms by either the band or profile scheme comprises a large fraction of the total storage. Thus, a compact storage scheme, which stores only the non-zero coefficients of a matrix provides a substantial reduction in core requirements for large systems.

The implementation of compact storage requires two integer array vectors, say ISTART and NAME, and a vector of the non zero coefficients, say AA. The i th integer entry in ISTART is the number q_i, where

$$q_i = \sum_{j=1}^{i-1} P_j + 1 \qquad (10)$$

and P_i is the number of terms in the j th equation (i.e. the number of nodes connected to the j th node). In n is the number of unknowns in the system, the length of ISTART is (n + 1). ISTART then, is a pointer vector whose j^{th} term locates the initial position in the AA vector of the contributing coefficients to the j^{th} equation. The M x 1 NAME vector, where

$$M = \sum_{j=1}^{n} P_i \qquad (11)$$

is composed of n successive vector blocks of variable length P_j: The P_j integers in the j^{th} block of NAME identify the contributors to the j^{th} equation. The M x 1 vector AA, contains the real non-zero coefficients of the n x n A matrix, arranged in the same contiguous block arrangement as the NAME vector.

A comparison of the core requirements of a symmetric banded matrix using banded, profile and compact storage follows. To fix ideas, we consider a simple rectangular domain with R rows of elements, and S columns of elements. The class of triangular elements with polynomial interpolation are considered. The formulas presented are for the case where interior nodes are condensed out. The following notation is used.

n - the number of unknowns

n_s - the half bandwidth for a symmetric matrix

t - the order of polynomial interpolation

R - the number of rows of elements in the rectangular grid

S - the number of columns of elements in the rectangular grid

N_s - symmetric band storage

N_p - profile storage

N_c - compact storage

α - bytes per word for real numbers

β - bytes per word for integer numbers

To obtain minimum bandwidth, numbering of nodes is sequential in the vertical direction if R < S, and vice versa if S > R, for profile and banded storage. The numbering sequence for compact storage is irrelevant. For an R x S rectangular grid the number of unknowns is

$$n = RS(3t - 2) + (R + S)(2 - 2t) + (t - 1) \qquad (12)$$

For very large systems, i.e. RS >> (R + S),

$$n \simeq RS(3t - 2) \qquad (13)$$

The core requirement for each of the storage schemes, for R < S, is

a) banded storage

$$N_s = \alpha n n_s \qquad (14)$$

where,

$$n_s = 3Rt - 2R - t + 3 \qquad (15)$$

For very large systems

$$\begin{aligned} N_s &\simeq \alpha R^2 S && \text{for } t = 1 \qquad (16)\\ N_s &\simeq 16\alpha R^2 S && \text{for } t = 2\\ N_s &\simeq 49\alpha R^2 S && \text{for } t = 3 \end{aligned}$$

b) profile storage

$$N_p = N_S - \alpha Q \qquad (17)$$

where

$$Q = \frac{(R-2)(R-1)}{2}t^2 + (R-2)(R-1)(t-1)t\,(S-1) + \frac{(R-2)(t-1)t(S-1)}{2} + \frac{[2R(t-1)+1][2R(t-1)+2]}{2}(S-2) \qquad (18)$$

For very large systems

$$\begin{aligned} N_p &\simeq \alpha R^2 S && t = 1\\ N_p &\simeq 12\alpha R^2 S && t = 2 \qquad (19)\\ N_p &\simeq 35\alpha R^2 S && t = 3 \end{aligned}$$

c) compact storage

$$N_c = \alpha M + \beta(M + n + 1) \qquad (20)$$

where

$$M = RS(15t^2 - 6t - 2) + (R + S)(-14t^2 + 8t + 2) \qquad (21)$$
$$+ (13t^2 - 10t - 1)$$

For very large systems

$$\left.\begin{array}{ll} N_c \simeq RS(7\alpha + 8\beta) & t = 1 \\ N_c \simeq RS(46\alpha + 50\beta) & t = 2 \\ N_c \simeq RS(115\alpha + 122\beta) & t = 3 \end{array}\right\} \qquad (22)$$

d) Comparison of N_s, N_p and N_c for large systems.

It is noted that banded and profile storage are proportional to R^2S, while compact storage is proportional to RS. The following formulas compare the relative core requirements for banded, profile and compact storage schemes.

i) Savings of profile compared to banded storage

$$\frac{N_s - N_p}{N_s} \simeq \left\{\begin{array}{ll} 0.0 & t = 1 \\ 0.25 & t = 2 \\ 0.29 & t = 3 \end{array}\right. \qquad (23)$$

ii) Savings of compact compared to profile

$$\frac{N_p - N_c}{N_p} \simeq \left\{\begin{array}{ll} 1 - \frac{7}{R} - \frac{8\beta}{\alpha R} & t = 1 \\ 1 - \frac{23}{6R} - \frac{25\beta}{6\alpha R} & t = 1 \\ 1 - \frac{23}{7R} - \frac{122\beta}{35\alpha R} & t = 3 \end{array}\right. \qquad (24)$$

To fix ideas, say $\beta = \frac{1}{2}\alpha$, then for large systems

$$\frac{N_p - N_s}{N_p} \simeq \begin{cases} 1 - \frac{11}{R} & t = 1 \\ 1 - \frac{71}{12R} & t = 2 \\ 1 - \frac{352}{70R} & t = 3 \end{cases} \qquad (25)$$

It should be noted from Eq. (24), that banded and profile storage is less than compact storage for small systems. For example, in the case of t = 1, banded and profile storage is more efficient when $1 < (\frac{7}{R} + \frac{8\beta}{\alpha R})$, i.e., when $R < 11$ in the case $t = 1$ and $\beta = \alpha/2$.

4. Numerical Results for an Example Problem

We consider the example given by Eq. (7), resulting in the ordinary differential equations (8). The domain was a rectangle which was discretized with 11 rows and 12 columns, giving 132 nodes and 220 elements. There were 22 boundary nodes (fixed values). Using linear triangular elements, a system of 110 differential equations was obtained. The three dimensional array (C_{ijk}) required special consideration for its storage. We noted that $\sum_{j=1}^{n} \sum_{k=1}^{n} C_{ijk}\gamma_j\gamma_k = \sum_{j=1}^{n} \sum_{k=j}^{n} D_{ijk}\gamma_j\gamma_k$

where

$$D_{ijk} = \begin{cases} C_{ijk} & j = k \\ C_{ijk} + C_{ikj} & j < k \end{cases} \qquad (26)$$

Because of the regular rectangular grid employed here, each equation contains no more than 7 tems. To facilitate handling of the nonlinear term, seven entries were allotted to each block of the NAME array (i.e. $P_j = 7$ for all j). For equations with q contributing terms, where $q < 7$, there were $(7 - q)$ null entries in the NAME array. For the nonlinear term given by Eq. (26), the number of non zero coefficients in any equation is no more than 28, the number of combinations of seven nodes taken two at a time (i.e. $C_{ijk} + C_{ikj}$, $j < k$) plus the seven diagonal terms C_{ijj}. Thus, the nonlinear term requires 28n words. Each of the (A_{ij}) and (B_{ij}) matrices requires 7n words. Total level 1 storage required is $42n\alpha$ bytes plus $7n\beta$ bytes for the NAME array; the ISTART array is not required for this modified compact storage scheme.

The J matrix that arises in this problem is $(\frac{s}{h}A_{ij} - bA_{ij} + cB_{ij} + 2a\sum_{k=1}^{n} C_{ijk}\gamma_k)$. The matrix can be stored in compact form using the same NAME array as for (A_{ij}).

Three different linear equation solvers were considered, along with their associated storage schemes for J. The first was the IMSL pair LUDAPB/LUELPB for matrices in symmetric banded storage form. The half bandwidth for our sample problem was 12, thus in this case $12n = 1320$ words were required. No additional working storage is required by LUDAPB since it performs an in-place decomposition of J. In the general case, storage requirements for the J matrix are those for a symmetric banded matrix as given by Eqs. (14) and (15).

The second equation solver used was an iterative method, SOR, for which compact storage was used. This required $7n = 770$ words. In general., storage requirements for the J matrix in compact form are given by Eq's (20 and (21). SOR, of course, does not require any additional working storage.

The third equation solver considered was the symmetric form of the Yale Sparse Matrix Package [4]. This required J to be stored in a symmetric form of the compact storage described in Section 3, and for our case required 399 words to store J, plus 510 words to store the NAME and ISTART arrays. In addition, approximately 1500 words were required to store the decomposition of J, along with the NAME and ISTART arrays. In general, storage for the Yale Sparse Matrix Package should be much less than that for the profile scheme given by Eqs (17) and (18), since a reordering of rows/columns to minimize fill-in during the matrix factorization is done.

The particular problem we have used as an example was designed to illustrate the feasibility of using the three different storage/solution schemes, and the computational times and storage here are not likely to be representative of what might happen in larger problems. In particular, the relatively small bandwidth favors the symmetric band storage mode in computational effort.

The SOR method must converge very rapidly to be competitive in computational effort, since about 7n operations are required per iteration, whereas about $2n_s n$ (after factorization of J) are required for solution with symmetric banded matrices of half bandwidth n_s. Somewhat fewer operations are required for the Yale Sparse Matrix Package. For our case, SOR requires more computational effort than direct methods when the number of iterations for convergence exceeds 4 (i.e. when $7nN_I > 2n_s n$, where n_s is 12 and N_I is the number of iterations), although this is offset by the need to factor J each time it is recomputed. Since the solution $\delta\gamma$ of the system $J\partial\gamma = \rho$ method increments for the corrector equation, the accuracy requirements are low, and SOR requires few iterations for convergence. The results of our example should be observed with the above considerations in mind. All times were obtained on the IBM 360 model 67, using the Fortran H compiler.

rms accuracy required in Gears Method	LUDAPB/LUELPB	YALE	SOR
.1	30.0	34.8	26.2
.01	48.7	47.1	50.1
.001	66.6	71.0	57.0

Table 1

For systems with large bandwidths, we expect the computational effort required for both the Yale Sparse Matrix Package and SOR to be superior to the symmetric banded scheme.

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